Sebacic acid, butyl 1-phenylpropyl ester

Inchi: InChI=1S/C23H36O4/c1-3-5-19-26-22(24)17-13-8-6-7-9-14-18-23(25)27-21(4-2)20-15-11
InchiKey: BJBMGGLRVYELHP-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-215.09	kJ/mol	Joback Method
hf	-776.40	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.145		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	904.46	K	Joback Method
tc	1110.21	K	Joback Method
tf	504.71	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.07	J/mol×K	904.46	Joback Method
cpg	1131.01	J/mol×K	1075.92	Joback Method
cpg	1119.07	J/mol×K	1041.63	Joback Method
cpg	1105.94	J/mol×K	1007.34	Joback Method
cpg	1091.59	J/mol×K	973.04	Joback Method
cpg	1075.98	J/mol×K	938.75	Joback Method
cpg	1141.81	J/mol×K	1110.21	Joback Method
dvisc	0.0000320	Pa×s	904.46	Joback Method

dvisc	0.0000427	Pa×s	837.83	Joback Method
dvisc	0.0000600	Pa×s	771.21	Joback Method
dvisc	0.0000897	Pa×s	704.58	Joback Method
dvisc	0.0001459	Pa×s	637.96	Joback Method
dvisc	0.0002660	Pa×s	571.33	Joback Method
dvisc	0.0005680	Pa×s	504.71	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume